18 Monte Carlo Simulation of the Surface Structure of Ge on Si(001)

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Abstract. Large-scale Monte Carlo simulations are used to study the structural properties of small germanium islands on a silicon (001) surface. The interactions between particles are modeled using empirical potentials of the Stillinger–Weber and Tersoff forms. The suitability of the potentials for finite-temperature simulations of the Si(001) surface is examined and shortcomings are identified. The Ge islands on Si(001) show significant edge effects caused partly by the underlying substrate and to a lesser extent by lattice-mismatch induced strain in the islands.

18.1 Introduction

Mixed semiconductor systems have attracted great interest due to their important application possibilities in the microelectronic industry. The properties of germanium differ only slightly from those of silicon, which makes the Si-Ge system an ideal candidate for the study of mixed systems. The interesting phenomena related to surface reconstructions and strain relaxation involve length scales far beyond the reach of ab initio methods. Valuable insight into these otherwise intractable problems can be gained by using classical interatomic potentials in connection with large-scale simulations. Equilibrating semiconductor systems with complicated energy landscapes requires highly efficient simulation techniques. We find the Monte Carlo (MC) method to be the most suitable tool for investigating the structure of mixed Si-Ge systems.

Large-scale constant-pressure Monte Carlo simulations are employed to study the atomic scale structure of small Ge islands on a Si(001) substrate. The islands are observed to display significant edge effects indicating possible splitting of the islands beyond certain critical size. The splitting is predicted to occur in the direction perpendicular to the Ge dimer bonds. Dimer formation and relaxation of the surface are also discussed from the computational point of view.

18.2 Simulation Method

The Ge/Si(001) system is modeled using a slab containing 16 or 20 layers with the surface size varying from 8×8 to 64×64 atoms. The simulation unit cell

is constructed along the [110], [1$\bar{1}$0] and [001] directions. Periodic boundary conditions are used in the x and y directions. In the simulations, the surfaces are initially given a 2×1 reconstruction or left bulk terminated. The structural energy of the system, E, is calculated from the atomic coordinates using the Stillinger–Weber (SW) potential [1] or one of the Tersoff potentials (T2 or T3) [2,3]. T2 and T3 are different parametrizations of the same functional form. Ge parametrization exists for the SW [4] and the T3 [5] models. At each MC step, we choose a particle at position $\boldsymbol{r}_i$ and attempt to displace it by a small amount to position $\boldsymbol{r}'_i$. The acceptance probability is given by the standard Metropolis form with the energy difference calculated using the structural energy E. After each particle in the system has been attempted, we randomly choose new linear sizes for the system (L'_x, L'_y, L'_z), slightly altered from the previous ones. The positions of the atoms are scaled by the relative change in the linear system size: $x' = xL'_x/L_x$, $y' = yL'_y/L_y$ and $z' = zL'_z/L_z$. The acceptance probability is again calculated using the Metropolis form, now using an effective Hamiltonian given by $H_{\text{eff}} = E - Nk_{\text{B}}T\ln(L_xL_yL_z)$ [4].

18.3 Comparison of Empirical Potentials

Originally, most of the empirical potentials designed for silicon were fitted to bulk properties leaving their applicability to surface studies questionable. Some comparative studies have been performed to test the strengths and limitations of the potentials (see e.g. [7]); however, most previous studies have concentrated exclusively on static or zero-temperature calculations. The motivation in our study is to examine the suitability of three widely used potentials, SW, T2 and T3, for finite-temperature simulations of the Si(001) surface.

Experimentally the Si(001) surface is observed to form a 2×1 reconstruction in which the surface atoms organize into parallel dimer rows [6]. For all three potentials, the formation of dimers is energetically favorable but in simulations the surface reconstructs to form only small domains of straight dimer rows separated by antiphase boundaries (dimer rows are shifted by one lattice constant relative to each other). The energy difference between a configuration with two antiphase domains (both 2×1 reconstructed) and an ideal 2×1 reconstruction is extremely small. Our simulations at $T = 0.05\,\text{eV}$ give the following values for *the energy difference per dimer row*: 0.20 eV for T2, 0.083 eV for SW, and −0.013 eV for T3. Thus the Tersoff potential T3 is found to favor the antiphase configuration over the experimentally observed 2×1 structure, which limits the suitability of this potential for simulation studies of the Si(001) surface.

In addition, the finite thickness of the simulation slab was found to influence the bulk properties of the system. The effects of the surface have generally been assumed to extend only a few atomic layers into the bulk, thus a 20-layer slab should be sufficiently thick to prevent the two surfaces

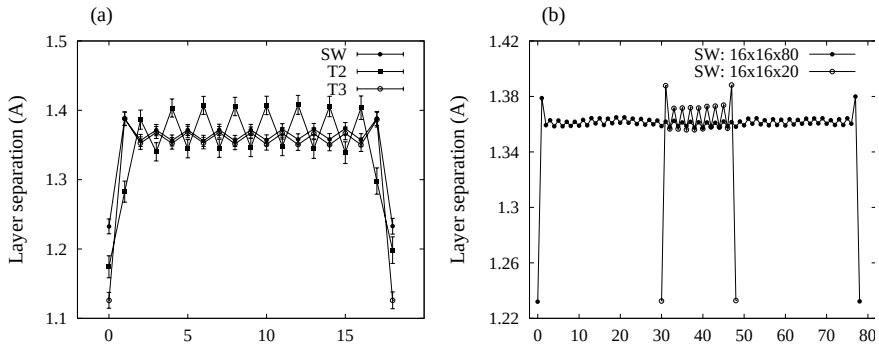

Fig. 18.1. Separation between atomic layers in the direction perpendicular to the (001) plane. (**a**) Comparison of different potentials. The system size is $16 \times 16 \times 20$ atoms. (**b**) Effect of slab thickness. The smaller slab has a thickness of 20 atomic layers and the larger slab 80 atomic layers. Temperature is 0.05 eV in both figures

from interacting with each other. Most measured quantities (average number of bonds, average bond length and bond angle, etc.) do reach a constant value starting approximately from the fifth substrate layer below the surface. However, we found that the average separation between atomic layers in the direction perpendicular to the (001) plane oscillates with a constant amplitude throughout the bulk. As can be seen from Fig. 18.1a, all three potentials produce similar oscillations, with SW and T3 giving identical results within statistical errors. Figure 18.1b shows that increasing the slab thickness reduces the amplitude of the oscillations. Such oscillations are not observed if periodic boundaries are imposed in all three directions, thus the oscillations are caused by the finite thickness of the slab. Surprisingly the amplitude does not decrease when moving toward the center of the slab, as would physically be expected of a surface effect. It should be noted that under the same conditions, T2 produces larger oscillations than T3 and SW. We know that the angular function of T2 is more flexible than those of T3 and SW [7]. This gives reason to believe that the inward relaxation of the first surface layer (which is in agreement with ab initio calculations [7]) produces a driving force for the oscillations that competes with the energy cost of distorting the bond angles and bond lengths. Thus careful attention should be paid to the selection of the potential and to its limitations when interpreting the results.

18.4 Ge Islands on Si(001)

As a physical application, we used the SW potential to study the relaxation of small Ge islands on a Si(001) surface. From experimental observations it is expected that islands larger than a certain critical size break apart due to growing strain in the island. Figure 18.2 shows the separation between

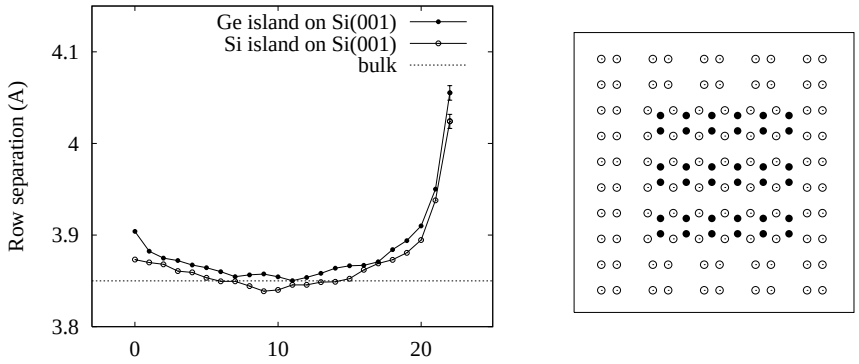

Fig. 18.2. Separation between dimer rows in the direction along the dimer bond for a Ge island (strained) and a Si island (unstrained) on Si(001). The size of the islands is 24×24 and the substrate size is 32×32. The atomic configuration of the island and first substrate layer is shown schematically on the right. The filled circles denote the top layer atoms (island) and the open circles atoms in the first substrate layer

vertical dimer rows (in the direction parallel to the dimer bonds) for a Ge island on Si(001) and a Si island on Si(001) at $T = 0.05\,\mathrm{eV}$. In both cases the island is square shaped with a size of 24×24 atoms. The Si substrate underneath has a surface size of 32×32 atoms. The atomic configuration of the island and first substrate layer is shown schematically (for a much smaller system) on the right in Fig. 18.2. The asymmetric form of the curves is an effect caused by the substrate dimers. When a substrate dimer row is directly bonded to an edge of the island (right edge of the island in Fig. 18.2), the substrate atoms "pull" the edge rows away from the island, which causes the island to spread in the direction of the substrate dimer bonds. The other edge of the island is not directly attached to a substrate dimer row, thus we do not observe such a pulling effect. At this end, however, the difference between the Ge island and the Si island becomes visible. The row separation in the Si island stays very close to the bulk value of 3.85 Å, while the Ge island spreads due to strain.

18.5 Conclusion

We have performed large-scale Monte Carlo simulations to study the surface structure of Ge on Si(001). Empirical interatomic potentials are used in the simulations because the phenomena we are interested in requires large system sizes reaching up to 10^5 particles. The suitability of the potentials for use in finite-temperature simulations of the Si(001) surface was investigated. The results show that some widely used potentials suffer from problems that can influence the outcome of the simulations significantly.

The SW potential was used to study the relaxation of small Ge islands on Si(001). The islands were found to display notable edge effects due to two different reasons. If one edge of the island is directly bonded to a substrate dimer row, the island expands due to pulling from the substrate dimers. Lattice-mismatch induced strain in the island also causes spreading in the same direction, but this effect is observed to be much weaker. However, these results give indication that the splitting up of very large islands occurs in the direction perpendicular to the Ge dimer bonds since even small islands show spreading in this direction. In on-going work we are developing more efficient simulation techniques to be able to address these issues in more detail.

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